

Time evolution operator

Let us consider a general approach that allows to determine (at least formally) how a state ket changes with time in the Schrödinger formulation of quantum mechanics. For simplicity we will assume that the Hamiltonian does not have any explicit dependence on time. Let us start with the time-dependent Schrödinger equation:

$$\frac{\partial \psi(\vec{r}, t)}{\partial t} + \frac{i\hat{H}}{\hbar} \psi(\vec{r}, t) = 0$$

We can multiply the equation from the left by the operator

$$\hat{U}^{-1} = \exp\left[\frac{i\hat{H}t}{\hbar}\right]$$

which is the inverse operator of $\hat{U} = \exp\left[-\frac{i\hat{H}t}{\hbar}\right]$. Recall that a function of an operator (e.g. the exponential one) is defined by its Taylor series. In our case

$$U^{-1} = 1 + \frac{i\hat{H}t}{\hbar} + \frac{1}{2!} \left(\frac{i\hat{H}t}{\hbar}\right)^2 + \frac{1}{3!} \left(\frac{i\hat{H}t}{\hbar}\right)^3 + \dots$$

After the multiplication by U^{-1} the Schrödinger equation can be written as

$$\frac{\partial}{\partial t} \left(\exp\left[\frac{i\hat{H}t}{\hbar}\right] \psi(\vec{r}, t) \right) = 0$$

which can be easily verified by differentiation of the product $\exp\left[\frac{i\hat{H}t}{\hbar}\right] \psi(\vec{r}, t)$.

Then we can integrate over the time interval $(0, t)$, which gives

$$\exp\left[\frac{i\hat{H}t}{\hbar}\right]\psi(\vec{r},t) - \psi(\vec{r},0) = 0$$

Now we can multiply it by \hat{U} from the left and obtain

$$\psi(\vec{r},t) = \exp\left[-\frac{i\hat{H}t}{\hbar}\right]\psi(\vec{r},0) = U\psi(\vec{r},0)$$

because $\hat{U}\hat{U}^{-1} = \exp\left[-\frac{i\hat{H}t}{\hbar}\right]\exp\left[\frac{i\hat{H}t}{\hbar}\right] = \hat{1}$, which can be verified by multiplying two Taylor series.

Operator U is called the time evolution operator. When we apply this operator to ψ at the initial time $t=0$ we obtain the wave function at time t . In fact, it is trivial to show that if we are given the wave function at $t=t_i$ then the the time evolution operator that yields the wave function at $t=t_f$ is

$$U(t_f, t_i) = \exp\left[-\frac{i\hat{H}(t_f - t_i)}{\hbar}\right]$$

i.e.

$$U(t_f, t_i)\psi(\vec{r}, t_i) = \psi(\vec{r}, t_f)$$

The time evolution operator gives a formally simple solution to a time-dependent problem. It has two important properties:

1. U is unitary, i.e. it preserves the normalization of the wave function (at least when \hat{H} is real)

$$2. U(t_2, t_1)U(t_1, t_0) = U(t_2, t_0) \quad (t_0 < t_1 < t_2)$$

It is possible to generalize to the case when

the Hamiltonian depends on time. We will give the corresponding expression without proof:

$$\hat{U}(t_f, t_i) = \hat{T} \exp \left[-\left(\frac{i}{\hbar}\right) \int_{t_i}^{t_f} H(t) dt \right]$$

where \hat{T} is the Dyson time ordering operator.

Alternatively it can be written as

$$U(t_f, t_i) = 1 + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 \int_{t_i}^{t_2} dt_3 \dots \int_{t_i}^{t_{n-1}} dt_n H(t_1) \dots H(t_n)$$

which is known as the Dyson series.

The above two expressions do not make any assumptions about $\hat{H}(t')$ commuting with $\hat{H}(t'')$. If, on the other hand \hat{H} is such that $[\hat{H}(t'), \hat{H}(t'')] = 0$ for any t' and t'' in the interval (t_i, t_f) then the time ordering operator can be dropped. Then

$$\hat{U}(t_f, t_i) = \exp \left[-\left(\frac{i}{\hbar}\right) \int_{t_i}^{t_f} H(t) dt \right]$$

Schrödinger, Heisenberg, and interaction pictures

Wave functions and operators themselves are not objects of measurements in quantum mechanics. Possible outcomes of a measurement are given by certain projection in Hilbert space. For example, if $\hat{A}|a\rangle = \alpha|a\rangle$ and the system is in state $|\psi\rangle$ the probability that a measurement of the observable corresponding to \hat{A} yields α is given by $|\langle a|\psi\rangle|^2$. This leaves room for alternative formulations (referred to as pictures) of quantum mechanics. Any picture must satisfy two basic requirements: i) Eigenvalues of operators corresponding to an observable must be the same as in the Schrödinger picture ii) inner products must have the same values as in the Schrödinger picture.

Previously we showed that (in the Schrödinger picture) the time evolution of the wave function is given by

$$|\psi_s(t)\rangle = \hat{U}(t,0) |\psi_s(0)\rangle$$

$$|\psi_s(0)\rangle = \hat{U}^{-1}(t,0) |\psi_s(t)\rangle$$

where index "s" stands for the Schrödinger picture.

Let us introduce $|\psi_H\rangle$, the wave function in the Heisenberg picture, as follows

$$|\psi_H\rangle = \hat{U}^{-1} |\psi_s\rangle \quad \hat{U} |\psi_H\rangle = |\psi_s\rangle$$

Then we can see that

$$|\psi_H\rangle = \hat{U}^{-1} |\psi_s(t)\rangle = |\psi_s(0)\rangle$$

That is, in the Heisenberg picture the wave function remains constant. On the other hand, operators, which in the Schrödinger picture are constant, vary in time:

$$\hat{A}_H(t) = \hat{U}^{-1}(t) \hat{A}_S \hat{U}(t)$$

An important exception is the Hamiltonian. If \hat{H} happens to be constant in the Schrödinger picture it remains constant in the Heisenberg picture.

As the wave function is time-independent in the Heisenberg picture, in order to determine how the system changes with time we need to obtain an equation of motion for $A_H(t)$. Let us take the derivative of A_H :

$$\frac{d\hat{A}_H}{dt} = \frac{d}{dt}(\hat{U}^{-1} \hat{A}_S \hat{U}) = \frac{d\hat{U}^{-1}}{dt} \hat{A}_S \hat{U} + \hat{U}^{-1} \frac{d\hat{A}_S}{dt} \hat{U} + \hat{U}^{-1} \hat{A}_S \frac{d\hat{U}}{dt}$$

If $\hat{A}_S = \hat{A}_S(\hat{p}_S, \hat{x}_S, t)$ we can say that

$$(*) \quad \frac{d\hat{A}_S}{dt} = \frac{\partial \hat{A}_S}{\partial t} \quad \text{because neither } \hat{p} \text{ nor } \hat{x} \text{ depend on time in the Schrödinger picture}$$

Now recall that $\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1) \hat{U}(t_1, t_0)$ $t_0 < t_1 < t_2$

Also let us recall the definition of differentiation:

$$\frac{d\hat{U}(t, 0)}{dt} = \lim_{\Delta t \rightarrow 0} \frac{\hat{U}(t + \Delta t, 0) - \hat{U}(t, 0)}{\Delta t}$$

This gives

$$\hat{U}(t + \Delta t, 0) = \hat{U}(t + \Delta t, t) \hat{U}(t, 0)$$

$$\text{and } \frac{d\hat{U}(t, 0)}{dt} = \lim_{\Delta t \rightarrow 0} \frac{[\hat{U}(t + \Delta t, t) - 1] \hat{U}(t, 0)}{\Delta t}$$

For sufficiently small Δt we may terminate the Taylor series for \hat{U} :

$$\hat{U}(t+\Delta t, t) = \exp\left[-\frac{i\hat{H}\Delta t}{\hbar}\right] \approx 1 - \frac{i\hat{H}\Delta t}{\hbar}$$

When we substitute it into the previous expression we get

$$i\hbar \frac{d\hat{U}}{dt} = \hat{H}\hat{U}$$

or, if we take the Hermitian adjoint

$$-i\hbar \frac{d\hat{U}^\dagger}{dt} = \hat{U}^\dagger \hat{H}$$

These last two equations can then be substituted into (*), which gives

$$i\hbar \frac{d\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}_H] + i\hbar \frac{\partial \hat{A}_H}{\partial t}$$

where we have set $\frac{\partial \hat{A}_H}{\partial t} \equiv \hat{U}^{-1} \frac{\partial \hat{A}_S}{\partial t} \hat{U}$

In addition to the Heisenberg picture one may also think of the so called interaction picture that can be useful in the situations when the Hamiltonian consists of two parts - one is time independent while the other depends on time, e.g.

$$\hat{H} = \hat{H}_0 + \hat{V}(t)$$

The interaction picture is kind of an "intermediate" between the Schrödinger and the Heisenberg pictures. The wave function in the interaction picture is given by

$$\Psi_I = \hat{U}_0^{-1} \Psi_S \quad \text{where} \quad \hat{U}_0 = \exp\left[-\frac{i}{\hbar} \hat{H}_0 (t_f - t_i)\right]$$

For operators we have

$$\hat{A}_I = U_0^{-1} \hat{A}_S U_0$$

Taking the time derivative of $\Psi_I = U_0^{-1} \Psi_S$ and noting that $[\hat{U}_0, \hat{H}_0] = 0$ one can obtain the equation of motion:

$$i\hbar \frac{\partial \Psi_I}{\partial t} = \hat{V}_I \Psi_I$$

which looks similar to the Schrödinger equation but only involves the time-dependent part of the Hamiltonian (usually that is the interaction potential). Integrating the above equation gives

$$\Psi_I(t) = \Psi_I(0) + \frac{1}{i\hbar} \int_0^t \hat{V}_I(t') \Psi_I(t') dt'$$

This equation is convenient for seeking the solution as a series. Substituting $\Psi_I(t)$ given by the right-hand side in the integrand and continuing such iterations generates the series

$$\Psi_I(t) = \Psi_I(0) + \frac{1}{i\hbar} \int_0^t dt' \hat{V}_I(t') \Psi_I(0) + \left(\frac{1}{i\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \hat{V}_I(t') \hat{V}_I(t'') \Psi_I(0) + \dots$$